

=> d his

(FILE 'HOME' ENTERED AT 06:34:18 ON 25 NOV 2002)

FILE 'CA' ENTERED AT 06:34:30 ON 25 NOV 2002

L1 2373516 S MIXTURE OR MIXED OR MIXING OR MIX  
L2 99211 S DATABASE OR DATA BASE OR LIBRARY  
L3 584065 S STANDARD OR CALIBRAT?  
L4 4213 S L1 AND L2  
L5 75121 S L1 AND L3  
L6 391 S L4 AND L5  
L7 2488078 S GRAPH? OR MODEL? OR DISPLAY? OR REPRESENT? OR DIAGRAM  
L8 444110 S L7 AND(TEMP OR TEMPERATURE OR DEG)  
L9 73451 S L1-3 AND L8  
L10 33 S L6 AND L9  
L11 141 S L6 AND(LIQUID OR FLUID OR SOLUTION OR AQUEOUS OR WATER OR H2O)  
L12 139476 S TITRATE# OR TITRANT OR TITRATION OR TITRATING  
L13 178081 S L1(3A) (PREPAR? OR FORM? OR MAKE)  
L14 16857 S L1(5A) (PLURAL? OR MULTI? OR ARRAY OR LIBRARY)  
L15 1306 S L13 AND L14  
L16 9 S L12 AND L15  
L17 552 S L15 AND(LIQUID OR FLUID OR SOLUTION OR AQUEOUS OR WATER OR H2O)  
L18 48 S L17 AND(REPLAC? OR REMOV?)  
L19 15 S L17 AND L3  
L20 34 S L8 AND L17  
L21 51852 S L1 AND REFERENCE NOT L5  
L22 369 S L4 AND L21  
L23 20 S L22 AND L8  
L24 112 S L22 AND(LIQUID OR FLUID OR SOLUTION OR AQUEOUS OR WATER OR H2O)  
L25 381 S L10-11,L16,L18-20,L23-24  
L26 252 S L25 NOT PY>1998  
L27 4 S L25 AND PATENT/DT NOT L26 AND PY<1999  
L28 256 S L26-27

=> d bib,ab 1-256 128

**L28** ANSWER 23 OF 256 CA COPYRIGHT 2002 ACS

AN 129:193625 CA

TI Considerations on the potentiometric log P determination

AU Kramer, Stefanie D.; Gautier, Jean-Claude; Saudemon, Philippe

CS Pharmaceutical Sciences Department. Sanofi Recherche, Montpellier, Fr.

SO Pharmaceutical Research (1998), 15(8), 1310-1313

AB A complementary approach to the existing calcn. program to calc. log P values from the **titrated** aq. pKa and the apparent pKa values (pKaapp) in biphasic systems. The presented data anal. method can be used for all kinds of protonable and deprotonable mols. like monoprotic and **multiprotic** acids and bases, **mixed** functional, and zwitterion **forming** compds. It permits an accurate evaluation of the results, which is not always evident when using the complex calcn. program delivered with the instruments.

**L28** ANSWER 61 OF 256 CA COPYRIGHT 2002 ACS

AN 126:270592 CA

TI The structure of mesophases of binary and **multicomponent mixtures** of some cholesteric **liquid** crystals

AU Obadovic, Dusanka Z.; Vajda, Aniko; Katona, Tibor Toth; Marinkovic - Neducin, Radmila

CS Institute of Physics, Faculty of Sciences, Novi Sad, Yugoslavia

SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1995), 265(Proceedings of the 15th

International Liquid Crystal Conference, 1994, Pt. 5), 2701-2707  
AB Binary and **multicomponent mixts.** of cholesteryl enanthate with cholesteryl nonanoate and cholesteryl formate were studied. The aim of the study is the prepn. of the system with phase transition **temp.** close to room **temp.** Phase **diagrams** of binary **mixts.** are **formed** from data obtained by the optical microscopy and DS calorimetry and the shift of phase transition points of order 30-50° with respect to initial components was established. In the case of three- and four-component mixts., the presence of enantiomorphic phase transitions of smectic and cholesteric type, resp. was identified. X-ray diffraction data have enabled the characterization of the structure of smectic or cholesteric mesophase and the calcn. of mol. parameters: apparent length of the mols. **l** and the av. intermol. distance (**D**).

L28 ANSWER 66 OF 256 CA COPYRIGHT 2002 ACS

AN 126:214574 CA

TI Modeling of the solubility of a one-component **H2O** or **CO2** fluid in silicate **liquids**

AU Papale, Paolo

CS Cent. Studio Geos logia Strutturale Dinamica Appennino, Pisa, I-56126, Italy

SO Contributions to Mineralogy and Petrology (1997), 126(3), 237-251

AB The modeling of the soly. of **water** and carbon dioxide in silicate **liqs.** (flash problem) is performed by assuming mech., thermal, and chem. equil. between the **liq.** magma and the gas phase. The **liq.** phase is treated as a **mixt.** of ten silicate components + **H2O** or **CO2**, and the gas phase as a pure **H2O** or **CO2**. A general model for the soly. of a volatile component in a **liq.** is adopted. This requires the definition of a **mixing** equation for the excess Gibbs free energy of the **liq.** phase and an appropriate ref. state for the dissolved volatile. To constrain the model parameters and identify th most appropriate form of the soly. equations for each dissolved volatile, a large no. of exptl. soly. detns. (640 for **H2O** and 263 for **CO2**) have been used. These detns. cover a large region of the P-T-compn. space of interest. The resultant **water** and carbon dioxide soly. models differ in that the **water** model is regular and isometric, and the carbon dioxide model is regular and non-isometric. This difference is consistent with the different speciation modalities of the two volatiles in the silicate **liqs.**, producing a compn.-independent partial molar volume of dissolved **water** and a compn.-dependent partial molar volume of dissolved carbon dioxide. The **H2O** soly. model may be applied to natural magmas of virtually any compn. in the P-T range 0.1 MPa-1 GPa and > 1000 K, whereas the **CO2** soly. model may be applied to several GPa pressures. The general consistency of the **water** soly. data and their relatively large no. as compared to the **calibrated** model parameters (11) contrast with the large inconsistencies of the carbon dioxide soly. detns. and their low no. with respect to the **CO2** model parameters (22). As a result, most of the soly. data in the **database** are reproduced within 10% of approxn. in the case of **water**, and 30% in the case of carbon dioxide. When compared with the exptl. data, the **H2O** and **CO2** soly. models correctly predict many features of the satn. surface in the P-T-compn. space, including the change from retrograde to prograde **H2O** soly. in albitic **liqs.** with increasing pressure, the so-called alkali effect, the increasing **CO2** soly. with increasing degree of silica undersatn., the Henrian behavior of **CO2** in most silicate **liqs.** up to about 30-50 MPa, and the proportionality between the fugacity in the gas phase, or the satn. activity in the **liq.** phase, and the square of the mole fraction of the dissolved volatile found in some unrelated silicate **liq.** compns.

L28 ANSWER 89 OF 256 CA COPYRIGHT 2002 ACS

AN 124:218999 CA  
TI A simple method for the **titration** of **multicomponent** acid-base mixtures  
AU Toisio, T.; Heikonen, M.  
CS Valio Ltd., Helsinki, FIN-00370, Finland  
SO Fresenius' Journal of Analytical Chemistry (1996), 354(3), 271-7  
AB A **titrn.** method was developed to analyze acid mixts., in which the pK values differed by 0.5 to 1 pH units. Instead of the use of equivalence points a buffer capacity curve is numerically derived from the **titrn.** curve resulting in a presentation similar to chromatograms and spectra. The consumption of the NaOH **titrant** is detd. within pH intervals of 0.2-0.6 units around the pK values of the components. The buffer capacity measured is expressed as the consumption of NaOH over the pH interval. The amts. of compds. are found from these results using simple models of chemometrics. The method was applied to a **mixt.** of **formic** and acetic acids with concns. of 0-3 mmol/20 mL with an error of 0-0.05 mmol. Also a curve-fitting method based on a theor. equation of buffer capacity can be applied with an error slightly larger than with the previous method. In this case, the pK values were also computed. For **titrns.** beyond the pH range 4-10, the buffer capacity of H2O has to be subtracted from the **titrn.** results. The whole procedure requires including the computations ~3-6 min.

L28 ANSWER 93 OF 256 CA COPYRIGHT 2002 ACS  
AN 124:157363 CA  
TI Thermodynamics of **aqueous** electrolytes at high **temperatures** by the isopiestic technique  
AU Holmes, H. F.; Mesmer, R. E.  
CS Chemical and Analytical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831-6110, USA  
SO Physical Chemistry of Aqueous Systems: Meeting the Needs of Industry, Proceedings of the International Conference on the Properties of Water and Steam, 12th, Orlando, Fla., Sept. 11-16, 1994 (1995), Meeting Date 1994, 533-40. Editor(s): White, Howard J., Jr. Publisher: Begell House, New York, N. Y.  
AB Excess thermodyn. properties of a wide variety of **aq.** electrolyte **solns.** at elevated **temps.** were detd. with the ORNL high-**temp.** isopiestic facility. This unique exptl. app. provides very precise results over the useful **temp.** range of 110-250°. The isopiestic method is a comparative technique which, in the present case, uses the Pitzer-Peiper-Busey formulation for NaCl(**aq**) as the **ref.** electrolyte. At elevated **temps.** the ion-interaction **model** of Pitzer continues to be the most useful description of the exptl. results. The exptl. program included the alkali metal chlorides, sulfates, hydroxides, bromides, and bisulfates, the alk. earth metal chlorides, and several specific compds. of scientific and practical interest. Numerous common-ion **mixed** electrolyte **solns.** were also investigated in this program. In general, the activity coeffs. of all the studied electrolytes decrease with increasing **temp.** However, prominent differences between members of the same family remain, particularly when considered as the excess Gibbs free energy. The tendency for ion assocn. increases with increasing **temp.** and becomes a factor at the higher **temps.** Trends and specific effects are illustrated with examples taken from the **database** generated in our high-**temp.** thermodyn. program.

L28 ANSWER 108 OF 256 CA COPYRIGHT 2002 ACS  
AN 122:70730 CA  
TI Qualitative analysis in the near-infrared region  
AU Downey, Gerard  
CS Dep. Plant Marine Foods, Natl. Food Cent., Dublin, UK  
SO Analyst (Cambridge, United Kingdom) (1994), 119(11), 2367-75

AB A review, with 29 refs., provides an up-to-date overview of the chemometric approaches available to users of near-IR spectroscopy specifically for the **soln.** of qual. anal. problems. The problems addressed include discrimination between similar materials of different functional classes; identification of pure chems. using a previously established spectra **library**; selection of optimum **calibration** sample sets with detection of outlying and redundant samples; and preliminary studies into the anal. of **mixts.** Among procedures discussed are discriminant methods (both supervised and unsupervised) and pattern recognition techniques.

**L28** ANSWER 152 OF 256 CA COPYRIGHT 2002 ACS

AN 115:84579 CA

TI Experimental methods for determining the eutectic composition of a **multi-component liquid crystal mixture**

AU Margerum, J. David; Van Ast, Camille I.; Myer, Gary D.; Smith, Willis H., Jr.

CS Hughes Res. Lab., Malibu, CA, 90265, USA

SO Molecular Crystals and Liquid Crystals (1991), 198, 29-36

AB Exptl. techniques are described for detg. the eutectic compn. of **multicomponent mixts.** of nematic **liq.** crystals. These techniques were applied to the formulation of nematic esters, when the idealized eutectic compn. calcd. by the Schroeder-Van Laar relationship did not give a good m.p. min. for the mixt. One exptl. procedure was based on the assumption that the compn. of the initial nematic melt from a frozen, crystd. mixt. is closer to a true eutectic than is the calcd. value from which the frozen **mixt.** was **formulated.** Another exptl. procedure was based on the assumption that a new eutectic could be obtained by **adding small amts.** of a new component to an existing **multi-component eutectic mixt.,** using the plot of the m.p. vs. the percentage of the new component added to det. a new eutectic mixt. corresponding to a new m.p. min. High performance **liq.** chromatog. was used to est. the purity of each component, and to analyze quant. the component compn. of each melt. The **calibration** plots for each **liq.** crystal component, as well as the chromatog. anal. of the mixts. are shown.

**L28** ANSWER 169 OF 256 CA COPYRIGHT 2002 ACS

AN 111:239373 CA

TI Calorimetric determination of **mixing** energies in **multicompartment** systems. Part 1: Construction of a **titration** calorimeter and interpretation by means of the deconvolution of the measuring function

AU Mueller, B. W.; Franzky, H. J.

CS Christian-Albrechts Univ., Kiel, Fed. Rep. Ger.

SO Pharmazie (1989), 44(7), 462-6

LA German

AB Microemulsions (esp. pharmaceutical) contg. surfactants, cosurfactants, oil, and **water** form oil-in-**water** and **water**-in-oil emulsions if they are dispersed systems and not colloidal **solns.** The study deals with the construction of a **titrn.** calorimeter and detn. of mixing enthalpies of a 2-component system by means of the deconvolution of the measuring function. A detailed scheme for the calorimeter construction, its **calibration** aspects and free mixing enthalpy of ethoxylated glycerol monostearate-H<sub>2</sub>O systems are discussed.

=> log y

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=> d his

(FILE 'HOME' ENTERED AT 13:24:35 ON 25 NOV 2002)

FILE 'CA' ENTERED AT 13:24:44 ON 25 NOV 2002

L1 36849 S (ADD? OR INJECT?) (2A) (AMOUNTS OR PORTIONS OR VOLUMES) OR (MULTIPLE OR  
SEVERAL OR PLURAL?) (3A) (ADDITIONS OR INJECTIONS)  
L2 18454 S L1 AND (MIXTURE OR MIXED OR MIXING OR MIX OR SOLUTION)  
L3 694 S ((ADD? OR INJECT?) (2A) (AMOUNTS OR PORTIONS OR VOLUMES) OR (MULTIPLE OR  
SEVERAL OR PLURAL?) (3A) (ADDITIONS OR INJECTIONS)) / TI, ST, IT  
L4 167 S L2 AND L3  
L5 55 S L4 AND (PROPERTY OR STEPWISE OR STEP WISE)  
L6 112 S L4 NOT L5  
L7 4 S L6 AND (CHCL3 OR STANDARD ADDITION OR REFRACTIVE INDEX)  
L8 168 S L1 AND (STEPWISE OR STEP WISE OR GRADIENT OR STANDARD) (2A) (ADDITION  
OR INJECTION)  
L9 72 S L8 AND (CALIBRAT? OR PARALLEL OR TITRANT OR TITRAT? OR (ELECTRODE OR  
CONCENTRAT? OR HANDLING) / TI)  
L10 121 S L5, L7, L9  
L11 106 S L10 NOT PY>1998

=> d bib, ab 1-106 l11

L11 ANSWER 2 OF 106 CA COPYRIGHT 2002 ACS

AN 128:123233 CA

TI Asymmetric distribution of results in **calibration** curve and **standard addition** evaluations

AU Renman, Lars; Jagner, Daniel

CS Analytical and Marine Chemistry, Department of Chemistry, University of Goteborg, S-412 96 Goteborg, Swed.

SO Analytica Chimica Acta (1997), 357(1-2), 157-166

AB The inherent asymmetry in the application of linear regression anal. to the detn. of sample analyte concns. using **calibration** curve or **std. addn.** evaluations gives rise to systematic errors. On the av., this always results in an overestimation of the true analyte concns. in **std. addn.** evaluations, while in **calibration** curve evaluations, the mean relative error depends on the value of sample concn. in relation to the analyte concns. used for the **calibration** curve. In both evaluation techniques, the distribution of the results will deviate from a Gaussian distribution even if all anal. signals are normally distributed. It is shown that, for the **std. addn.** technique and for samples with low analyte concns. evaluated by the **calibration** curve technique, optimum precision and accuracy is obtained by using a min. no. of **calibration** points or **std. addns.**, and performing **multiple** measurements on these. It is also shown that the linear regression correlation coeff. is a very poor indicator of the accuracy and precision in multiple-point **std. addn.** evaluations. Weighted linear regression can be used to decrease the magnitudes of the systematic errors, but due to the inherent asymmetry, the distribution of the results will nevertheless be non-Gaussian. A publically available, inhouse constructed Windows 3.1/Windows 95 program, capable of simulating all kinds of **calibration** curve and **std. addn.** evaluations, was used for all calcs.

L11 ANSWER 6 OF 106 CA COPYRIGHT 2002 ACS

AN 123:51462 CA

TI Determination of zinc in plasma by atomic absorption spectrometry with a graphite furnace and pyrolytic platform

AU Burrini, C.; Borghi, G.; Fuzzi, G.

CS Ist. Ricerche Clin., Florence, Italy

SO Giornale Italiano di Chimica Clinica (1994), 19(2), 127-31

AB We present a precise and accurate method for the detn. of zinc in blood

plasma by at. absorption spectrometry with graphite furnace and pyrolytic platform. The samples were dild. 40-fold with a 0.1% nitric acid and 0.025% Triton X 100 soln., six microliters of this diln. were utilized for the measurement. Zinc concns. were calcd. by comparison with a **calibration** curve prepd. by **adding** known **amts.** of a std. soln. to a dild. sample (**std. addns.** technique). The detection limit was 0.03 mg/L. Within-run CVs were 1.30% and 2.00% for plasma zinc concns. of 0.76 and 1.57 mg/L, while between-run CV was 3.86% for a concn. of 0.86 mg/L.

**L11** ANSWER 8 OF 106 CA COPYRIGHT 2002 ACS

AN 122:280756 CA

TI Validation of an analytical instrumental method by **standard addition** methodology

AU Rodriguez, Luis Cuadros; Campana, Ana M. Carcia; Barrero, Fermin Ales; Linares, Carlos Jimenez; Ceba, Manuel Roman

CS Fac. Sci., Univ. Granada, Granada, 18071, Spain

SO Journal of AOAC International (1995), 78(2), 471-6

AB A statistical procedure to validate an anal. methodol. by **std. addn.** methodol. is described. The data set obtained in 3 **calibration** expts. with **std. dilns.**, **std. addns.**, and **portions** of sample was used. The accuracy of the anal. results is checked by comparison of analyte contents in the different **calibrations** and from the recovery. Math. expressions to est. the statistical parameters are proposed. The statistical protocol was applied to fluorometric detn. of Mo with alizarin S in vegetable tissues.

**L11** ANSWER 19 OF 106 CA COPYRIGHT 2002 ACS

AN 115:196939 CA

TI In situ measurement of **electrode** slope and gravimetric multiple **standard addition** analysis by ion selective potentiometry without prior **calibration** of **electrode**

AU Chaudhuri, N. K.; Sawant, R. M.

CS Fuel Chem. Div., Bhabha At. Res. Cent., Bombay, 400 085, India

SO Analytical Letters (1991), 24(9), 1605-24

AB Two methods of calcn. for the detn. of an unknown concn. by gravimetric multiple **std. addn.** anal. using ion selective potentiometry without prior **calibration** of the electrode are described. These are based on simple calcn. procedures involving linear least square fitting to Gran's equation to evaluate first the actual electrode slope 'in situ', then the unknown concn. and the cell const. One method is iterative and the other is noniterative. The applicability of the methods is demonstrated by processing the exptl. data obtained by using fluoride and uranyl ion selective electrodes.

**L11** ANSWER 24 OF 106 CA COPYRIGHT 2002 ACS

AN 114:74518 CA

TI Linearized **multiple standard additions** for the potentiometric determination of weak acids

AU Macca, Carlo

CS Dep. Inorg., Organomet. Anal. Chem., Univ. Padova, Padua, I-35131, Italy

SO Talanta (1990), 37(12), 1141-9

AB The feasibility of potentiometric detn. of weak monoprotic acids by the multiple **std. addn.** method is examd. A std. **soln.** of pure weak acid is added to the **soln.** contg. an unknown amt. of the same weak acid, alone or **mixed** with its conjugate base. The exptl. data are processed by Gran-type plots, for which rigorous and approx. equations are obtained. It is shown that weak acids can be detd. by **multiple std. addns.** with a precision comparable with that of the usual kinds of potentiometric

addn. methods. The validity range of the approx. equations is established. Linear equations similar to those of Hofstee, Scatchard, Lineweaver and Burk, and Scott are also obtained, by which acidity consts. can be detd. together with equivalence vols. The effects of systematic and random measurement errors are examd.

L11 ANSWER 25 OF 106 CA COPYRIGHT 2002 ACS

AN 113:144237 CA

TI Preparation of solutions before **titration** by the **standard addition** technique

AU Zhukov, B. D.

CS Pac. Inst. Oceanol., Vladivostok, USSR

SO Zhurnal Analiticheskoi Khimii (1990), 45(6), 1167-72

AB A method is described for prepg. solns. for **titrn.** by the **std. addn.** method involving the soln. to be **titrated** and the **titrant** and including the distribution of the sample between them. Tests showed the effectiveness of such a prepn. on an example of ionometry during the development of conditions providing for minimal consumption of the indifferent electrolyte salt, independent of the vol. and the no. of addns. of such anal. characteristics as the compn. of the supporting electrolyte, the ionic strength, the slope of the electrode function, etc. In an example of detg. the F<sup>-</sup> concn. in aq. solns. by using the **multiple std. addns.** method with ion-selective electrodes, the equalization of the compns. and the value of the physicochem. characteristics of the soln. being **titrated** and the **titrant** also allow one to eliminate the influence of effects related to diln. of the soln. being **titrated**.

L11 ANSWER 27 OF 106 CA COPYRIGHT 2002 ACS

AN 112:110981 CA

TI Hybrid **multiple standard additions**-analyte **addition** method for ion-selective **electrodes** with integral **calibration**

AU Velinov, G.; Panushev, A.

CS Med. Acad., Sofia, 1000, Bulg.

SO Analyst (Cambridge, United Kingdom) (1989), 114(8), 929-32

AB A hybrid **multiple std. addns.**-analyte **addn.** method for ion-selective electrodes is described in which the **calibration** of the potentiometric cell and the detn. of the unknown concn. of the sample are carried out in a single expt. This ensures max. constancy of the **calibration** characteristics, E°' and S, of the cell. The proposed method allows the detn. of trace amts. (100 µg) of an analyte. The data treatment includes an iterative minimization procedure using the least-squares sum method, which improves the accuracy and the statistical reproducibility of the results. The method can be automated by means of an automatic **titrator**, controlled by an HP-85B microcomputer. A BASIC program was constructed for this purpose. The method was tested by applying it to the detn. of sodium, potassium, chloride and fluoride ions and the errors of the results were less than 1%. The detn. limit of the method was investigated by detg. decreasing concns. of fluoride ions. It was found that the method gives satisfactory results over the entire linear range of the ion-selective electrode.

L11 ANSWER 29 OF 106 CA COPYRIGHT 2002 ACS

AN 108:215482 CA

TI Method of **parallel** addition in ionometry

AU Urusov, Yu. I.; Tsygankov, A. M.; Zhukov, A. F.; Firer, A. A.

CS Moscow Chemicotechnol. Inst., Moscow, USSR

SO Zhurnal Analiticheskoi Khimii (1988), 43(3), 421-5

AB A new method for detg. anions in acid media is based on **addn.** of equal

vols. of a std. soln. with different analyte concns. to 2 **parallel** samples of equal vols. The effect of detn. conditions on the relative error has been examd. by taking  $\text{AuCl}_4^-$  and  $\text{PtCl}_6^{2-}$  as examples. The method is useful for the detn. of anions in solns. of different acid concn. by potentiometry with ion-selective electrodes.

~~L11~~ ANSWER 46 OF 106 CA COPYRIGHT 2002 ACS

AN 100:25847 CA

TI Automatic **titration** by **stepwise addition** of equal volumes of **titrant**. Part VIII. Determination of alkalinity and total carbonate in seawater

AU Johansson, Axel; Johansson, Sten; Gran, Gunnar

CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, S-100 44, Swed.

SO Analyst (Cambridge, United Kingdom) (1983), 108(1290), 1086-90

AB The reliability of a set of linear equations for the evaluation of **titrn.** data was investigated for the detn. of alky. and total  $\text{CO}_3^{2-}$  in seawater by potentiometric **titrn.** with std.  $\text{HCl}$  **soln.** The method requires that polyprotic acids be treated as a **mixt.** of monoprotic acids and approx. values for equil. consts. for the acid-base pairs is known. The results agreed well with those obtained by nonlinear curve-fitting methods.

~~L11~~ ANSWER 54 OF 106 CA COPYRIGHT 2002 ACS

AN 94:202069 CA

TI Automatic **titration** by **stepwise addition** of equal volumes of **titrant**. Part VI. Further extension of the Gran I method for calculation of the equivalence volume in acid-base **titrations**

AU Gran, Gunnar; Johansson, Axel

CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, S-10044/70, Swed.

SO Analyst (London) (1981), 106(1259), 231-42

AB The equivalence vol.,  $V_e$ , was calcd. from **titrn.** data by a method of **stepwise addn.** of equal vol. of **titrant** combined with an extended version of the Gran I method. The method can be used for monoprotic acids with  $\log K \leq 10$ . The  $V_e$  values for most di- and triprotic acids can also be calcd. by this method.

~~L11~~ ANSWER 56 OF 106 CA COPYRIGHT 2002 ACS

AN 93:211078 CA

TI Automatic **titration** by **stepwise addition** of equal volumes of **titrant**. Part V. Extension of the Gran I method for calculation of the equivalence volume in acid-base **titrations**

AU Johansson, Axel; Gran, Gunnar

CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, 10044/70, Swed.

SO Analyst (London) (1980), 105(1253), 802-10

AB The equiv. vol. is calcd. from **titrn.** data by a simple method based on **stepwise addn.** of equal vols. of **titrant** combined with an extension of the Gran I method. This method is also used to det. the conditional normal potential and the const. in the junction potential for an electrode couple in a given medium. **Titrens.** of very weak acids can not be evaluated by this method.

~~L11~~ ANSWER 58 OF 106 CA COPYRIGHT 2002 ACS

AN 92:33272 CA

TI High accuracy titrimetric analysis

AU Spivakovskii, V. B.; Dovgopol, O. S.; Makovskaya, G. V.; Moisa, L. P.

CS Inst. Met. Phys., Kiev, USSR

SO Zh. Anal. Khim. (1979), 34(9), 1681-6

AB A method for the detection of the deviation of the **titrn.** end point from



the equivalence point and for taking into account coordination of all anal. operations from the viewpoint of accuracy ensures high accuracy in the titrimetric detns. of macroconcns. of elements or the main components of substances to be analyzed. The method was tested on the titrimetric detn. of Pb in Pb(NO<sub>3</sub>)<sub>2</sub> of spectral purity with Complexon III at pH 4-8. The method involves **several std. addns.** of Pb, measurement of the a.c. polarog. peak current of Pb after each addn., and extrapolation of the curve obtained from these measurements.

L11 ANSWER 60 OF 106 CA COPYRIGHT 2002 ACS

AN 91:199756 CA

TI Automatic **titration** by **stepwise addition** of equal volumes of **titrant**. Part IV. General-purpose program for evaluating potentiometric acid-base **titrations**

AU Johansson, Axel; Johansson, Sten

CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, S-100 44/70, Swed.

SO Analyst (London) (1979), 104(1240), 601-12

AB A computer program, TITRA, for evaluating acid-base **titrn.** results, using nonlinear regression techniques, was studied. All n-protic acids were treated as a **mixt.** of n monoprotic acids of the same molality as the n-protic acid. The parameter calcns. were performed in an appropriate sequence. No preliminary ests. of the required concns. were necessary. The method was applied to samples of mono- and polyprotic acids, **mixts.** of acids, ampholytes, salts of weak acids, acids with an abnormal sequence of stability const. values, and bases. E.g., for a **mixt.** of HCl, phthalic acid, and barbital, the amts. found were 1.000, 0.9992 and 1.0055 mmol, resp., compared with 1.000, 1.0025 and 1.0011 mmol added, giving a recovery of 100.0, 99.7 and 100.4%, resp.

L11 ANSWER 61 OF 106 CA COPYRIGHT 2002 ACS

AN 90:214572 CA

TI Microcomputer-aided high-speed potentiometric **titration** system by linear **titration** plots

AU Yamaguchi, Shinichiro; Kusuyama, Takashi

CS Wakayama Res. Lab., Kao Soap Co., Ltd., Wakayama, Japan

SO Fresenius' Z. Anal. Chem. (1979), 295(4), 256-9

AB An app. for high-speed potentiometric **titrn.** was assembled and its advantage was demonstrated. **Titrant addns.** were made **stepwise** in large vols. The optimum increment vols. were automatically chosen by microcomputer, depending upon the sample concn. Time intervals between the successive addns. were controlled so as to add a new increment immediately after the electrode was equilibrated. On-line calcn. of the equivalence vol. was conducted based upon linear **titrn.** plots by using only 4 **titrn.** points before the equivalence point. The app. was capable of detg. the concn. of strong and weak monoprotic acids in <22 s with relative std. deviations of 0.1-0.2%.

L11 ANSWER 62 OF 106 CA COPYRIGHT 2002 ACS

AN 89:172898 CA

TI Automatic **titration** by **stepwise addition** of equal volumes of **titrant**. Part III. Use of linear equations to calculate equivalence volumes in acid-base **titrations**

AU Johansson, Axel; Johansson, Sten

CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, Swed.

SO Analyst (London) (1978), 103(1225), 305-16

AB A computational procedure is described for calcg. equivalence vols. for the **titrn.** of monoprotic acids, bases, and ampholytes with log K (K = stability const.) ≤11. The procedure is based on the **soln.** of a

set of linear equations and requires only a few sets of measurements of emf. vs. **titrant** vol. plus the initial vol. and **titrant** concn. Log K values are not required and emf. measurements may have a const. systematic error of  $\pm 6$  meV, corresponding to  $\pm 0.1$  pH unit. The program can automatically select appropriate measurements. Exptl. results had std. deviations  $< 0.2\%$ .

LI1 ANSWER 66 OF 106 CA COPYRIGHT 2002 ACS

AN 87:77978 CA

TI Acid-base **titrations** by **stepwise addition** of equal volumes of **titrant** with special reference to automatic **titrations**. IV. Photometric **titration** of an acid

AU Pehrsson, Lennart; Ingman, Folke

CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, Swed.

SO Talanta (1977), 24(2), 87-90

AB The method of **stepwise addn.** of **titrant** in acid-base **titrns.** (1977) is applied to photometric **titrn.** of monoprotic acids. The highest precision is obtained when the absorbance of the **titrn. mixt.** changes linearly with each addn. of **titrant**. For weak acids good results are found if the stability consts. of the acid and indicator differ by 0.3-0.5 logarithmic units. The method is tested on the **titrn.** of 0.01006M HCO<sub>2</sub>H with 0.1M NaOH and bromophenol blue indicator. Ten consecutive **titrns.** gave the concn. as 0.01007M with a coeff. of variation 0.12%. The advantages and disadvantages of the method are discussed.

LI1 ANSWER 67 OF 106 CA COPYRIGHT 2002 ACS

AN 87:77942 CA

TI Acid-base **titrations** by **stepwise addition** of equal volumes of **titrant** with special reference to automatic **titrations**. III. Presentation of a full automatic **titration** apparatus and of results supporting the theories given in the preceding parts

AU Pehrsson, Lennart; Ingman, Folke

CS R. Inst. Technol., Stockholm, Swed.

SO Talanta (1977), 24(2), 79-85

AB The title app. holds 200 sample tubes and performs the following operations; pipetting of sample and addn. of neutral salt to give const., high ionic strength; thermostatic temp. control to  $25 \pm 0.1^\circ$ ; addn. of **titrant** in equal vols. and detn. of the electrode potential after each addn.; rinsing of **titrn.** vessel and electrode couple; sample changeover. **Titrn.** results for monoprotic acids, e.g. HCO<sub>2</sub>H, HCO<sub>2</sub>H-EtCO<sub>2</sub>H **mixts.**, tartaric acid, K H phthalate, and HCO<sub>2</sub>H-HCO<sub>2</sub>-**mixts.** are given. These **titrns.** cannot be evaluated by the methods of G. Gran (1952) and B. H. J. Hofstee (1960) but the proposed method (1976) gives results accurate to 0.1%. The method is better than common **titrn.** methods in that all the data are used in the evaluation, permitting a statistical treatment.

LI1 ANSWER 68 OF 106 CA COPYRIGHT 2002 ACS

AN 86:182361 CA

TI Acid-base **titrations** by **stepwise addition** of equal volumes of **titrant** with special reference to automatic **titrations**. II. Theory of **titration** of **mixtures** of acids, polyprotic acids, acids in **mixture** with weak bases, and ampholytes

AU Pehrsson, Lennart; Ingman, Folke; Johansson, Sten

CS R. Inst. Technol., Stockholm, Swed.

SO Talanta (1976), 23(11-12), 781-8

AB A general method is given for evaluating **titrn.** data for **mixts.** of

acids, and for acids **mixed** with weak bases, which allows use of relative H concn. data, thus requiring only an approx. **calibration** of the elctrode system. For simple systems, only a rough calcn. of stability const. is required. Detailed example calcns. are given for **titrating** a binary acid **mixt.**, a diprotic acid, an acid-conjugate base system, and an ampholyte.

**L11** ANSWER 69 OF 106 CA COPYRIGHT 2002 ACS

AN 86:8518 CA

TI Determination of lead in saline water under use of flameless atomic-adsorption spectrophotometry

AU Kussmaul, H.; Majlis, S. K.

CS Frankfurt/Main, Ger.

SO Gas- Wasserfach, Wasser - Abwasser (1975), 116(12), 552-4

LA German

**AB** While estg. Pb in the water samples by means of the flameless atomic absorption spectrophotometry (graphite-pipe curvette), disturbances depending on the matrix compn. were obsd. It was evident that these were caused mainly by the Na in the surface waters. Other ions could cause signal depression or intensification. For elimination of these disturbances, an addnl. procedure was suggested, in which the **calibration** curve was plotted in a soln. with the same matrix compn. as that of the measuring soln. It occurred in this case by gradual **addn.** of the **std.** soln. to the water sample. A water sample 100 ml is acidified with concd. H<sub>2</sub>SO<sub>4</sub> 1 ml, known Pb **amts.** are **added** stepwise, and the respective extinction coeffs. are measured. *By this the necessity of a correction of the extinction depression was omitted, as the addn. procedure was equiv. to the plotting of the **calibration** curve of a soln. which contained the same matrix as the test sample.*

**L11** ANSWER 70 OF 106 CA COPYRIGHT 2002 ACS

AN 85:186166 CA

TI Automated computer-controlled solution **handling** system utilizing weights of solution

AU Renoe, B. W.; O'Keefe, K. R.; Malmstadt, H. V.

CS Sch. Chem. Sci., Univ. illinois, Urbana, Ill., USA

SO Anal. Chem. (1976), 48(4), 661-6

**AB** An automated sample and reagent soln. prepn. system, which is generally applicable in the anal. lab., was designed and tested. The new system utilizes an electronic sensor to weigh accurately the nominal aliquots of sample and reagent solns. that are added to a disposable beaker. Each plastic beaker on a turntable is automatically positioned on the wt. sensor. Reagent and sample solns. are added by gravity feed for selected time intervals to provide nominal amts. Each reagent or sample is accurately weighed after addn., and the beaker is then automatically moved to a stirring station while another beaker is moved into position for wt. measurements. The **amts.** of reagents **added** to the beaker can be incrementally adjusted as desired. The operational modes are specified by interaction through FORTRAN programming and FORTRAN callable subroutines, which control or accumulate data concerning the system turntable, wt. sensor, soln. delivery devices and mixer, and the computer peripherals. The anal. utility of the system is demonstrated by data obtained in automated prepn. of working curves and **std.-addn.** procedures.

**L11** ANSWER 73 OF 106 CA COPYRIGHT 2002 ACS

AN 79:73155 CA

TI Automated system for photometric **titration** by **stepwise** addition of equal **volumes** of **titrant**

AU Pehrsson, Lennart; Johansson, Axel  
CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, Swed.  
SO Anal. Chim. Acta (1973), 66(1), 67-74  
AB A completely automatic system for photometric **titrns.** delivers measured vols. of sample, indicator **soln.**, and buffer **soln.**, **titrates**, and finally rinses the **titrn.** vessels. **Titrns.** are performed by adding the **titrant** **stepwise** in equal vols. to the sample, measuring the absorbance after each addn., and calcg. the equivalence vols. The system performs ~30 **titrns./hr** and has a loading capacity of 200 samples. It was tested by **titrating** Ca with EGTA in presence of calmagite as indicator.

L11 ANSWER 81 OF 106 CA COPYRIGHT 2002 ACS

AN 73:126566 CA

TI Automatic **titration** by **stepwise addition** of equal volumes of **titrant**. II. Automatic **titration** system

AU Johansson, Axel; Pehrsson, Lennart.

CS Dep. Anal. Chem., Roy. Inst. Technol., Stockholm, Swed.

SO Analyst (London) (1970), 95(1132), 652-6

AB An automatic potentiometric **titrn.** app. pipets, dils., and **titrates** (by **addn.** of equal vols. of **titrant**) the sample and washes the electrodes and **titrn.** vessels, at a rate of  $\leq 30$  samples/hr. HCl (0.03354M) and 0.02293M HOAc in a binary **mixt.** were detd. by using the app. with + 0.00016M and -0.00017M abs. errors, resp., and with 0.2 and 0.9% relative std. deviations, resp.

L11 ANSWER 82 OF 106 CA COPYRIGHT 2002 ACS

AN 73:83501 CA

TI Computer approach to ion-selective **electrode** potentiometry by **standard addition** methods

AU Brand, Michael J. D.; Rechnitz, Garry A.

CS Dep. of Chem., State Univ. of New York, Buffalo, N. Y., USA

SO Anal. Chem. (1970), 42(11), 1172-7

AB Methods are described for detg. an unknown concn. by using an ion-selective electrode without prior **calibration** of the electrode. The methods are based on **std. addn.** procedures. In the simplest case, only 2 **std. addns.** are required and a simple calcn. is described which can be performed by a computing calculator. To obtain high accuracy in the detn. of unknown concns., **multiple addns.** are made and a least squares curve fitting method is used to evaluate the unknown concn., electrode slope, and std. potential. A computer program to accomplish this calcn., ADDFIT, is given in Fortran IV. The effectiveness of these methods is demonstrated by expts. on Pb and chloride samples.

L11 ANSWER 83 OF 106 CA COPYRIGHT 2002 ACS

AN 73:51898 CA

TI Automatic **titration** by **stepwise addition** of equal volumes of **titrant**. I. Basic principles

AU Johansson, Axel

CS Roy. Inst. Technol., Stockholm, Swed.

SO Analyst (London) (1970), 95(1131), 535-40

AB The basic principles of a potentiometric **titrn.** method, which is based on making potential measurements after each addn. of **titrant** in equal-vol. increments, are described. The method is esp. suitable for automation, e.g. in biochem. and process control anal. The method is demonstrated by NaOH **titrns.** of HCl and HOAc, both alone and in **mixts.**

L11 ANSWER 91 OF 106 CA COPYRIGHT 2002 ACS

AN 64:30996 CA  
OREF 64:5759f-h  
TI Phase **titrations**. V. Nitroalkanes. Improving the phase-**titration** end point  
AU Rogers, D. W.; Lillian, D.; Chawla, I. D.  
CS Am. School, Madrid  
SO Talanta (1966), 13(2), 313-18  
AB cf. CA 62, 12648f. End points for direct phase **titrns**. of binary solns.  
of nitropropanes in H2O-miscible solvents are fair and, because of the  
steepness of the **calibration** curve, results are adequate. EtNO2 ethane,  
in binary combination, gives poor end points but, over part of the optimum  
**titrn**. range, results are good. MeNO2 gives end points which are almost  
useless. **Addn.** of **standard amts.** of PhNO2, which gives excellent  
phase-**titrn**. end points, improves the composite MeNO2-PhNO2-H2O-miscible  
component end point markedly. Because the PhNO2 concn. is const., the H2O  
titer is a function only of the MeNO2 concn. **Addn.** of const. **amts.** of  
PhNO2 also increases the optimum **titrn**. range. Results given for all  
systems are comparable in accuracy with systems previously reported which  
are favorable to direct phase **titrn**.

=> log y

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